Comment on "Electronic fine structure in the electron-hole plasma of SrB_6"

In a recent Letter [1], Rodriguez *et al.* addressed the origin of the high-temperature weak ferromagnetism found in doped hexaborides [2] by calculating details of the band structure of SrB_6 in the vicinity of the X-point in the Brillouin zone. They conclude that crystal field induced electron-hole mixing has an important effect on the density of states (DOS) and suggest nesting between electron Fermi pockets as an alternative explanation to the excitonic ferromagnetism [3]. We would like to question several conclusions in this work [1].

(i) Rodriguez *et al.* claim that the two bands cross only along the symmetry lines $(\xi, 0, 0)$ and $(\frac{\pi}{a}, \xi, 0)$. This result contradicts a previous band structure study, which found band crossing in *all symmetry planes* passing through the X-point [4]. The latter conclusion has a simple symmetry interpretation. At the X-point the valence and conduction bands belong to different irreducible representations of the small group: X_3, basis function yz, and X_3' symmetry, basis function $x(y^2-z^2)$, respectively. The band mixing occurs away from the X-point and is given by the product $X_3 \times X_3'$

$$\Delta_{\rm cryst} \simeq E_b k_x k_y k_z (k_y^2 - k_z^2)/b^5 \ , \qquad (1)$$

where E_b is a bandwidth and $b = \frac{2\pi}{a}$ is a reciprocal lattice vector. The crystal field hybridization is strongly suppressed by the high power of momentum in Eq. (1) ($k_F \sim 0.1b$). Therefore, not only is the hybridization more anisotropic than suggested in Ref. [1], but also it is very weak on the scale of the band overlap. Our TB-LMTO calculations [3] as well as FLAPW method [5] yield an extremely small band mixing for a general direction in the Brillouin zone in agreement with Eq. (1).

(ii) Even for a strong hybridization, the DOS is quite different from the results of Ref. [1]. Fig. 1 shows the DOS for two parabolic bands with anisotropic effective masses [1,3], band overlap $E_G = 100$ meV, and two angular dependences for the mixing matrix element: isotropic, which models an excitonic gap [3], and anisotropic given by Eq. (1). The amplitudes were chosen to give the same maximum splitting of $2\Delta_{\rm max} = 15$ meV. Because of the anisotropic dispersion the DOS is slightly reduced at the Fermi level. The true gap in the DOS opens only for a sufficiently large excitonic gap $\Delta > 0.16 E_G$. Note that the tetrahedron method for DOS does not allow for crossing of bands, which are numbered in increasing order of energy at every k-point, and, therefore, may lead to spurious peaks [1] due to artificial anticrossings.

(iii) Correlation effects in the *e-h* plasma lead to a forbidden range for the band overlap values in the hexaborides [6]. At the first order metal-insulator transition a semiconductor jumps into a dense plasma with $r_s \approx 1$. Rodriguez *et al.* have estimated $r_s = 2.5$ for the band overlap $E_G = 100$ meV in SrB_6, a value lying within the forbidden range. The real overlap must be larger. Therefore, the conclusion that 0.5 % doping fills hole Fermi pockets in SrB_6 [1], which is based on the above underestimated value of E_G, is by no means reliable and does not exclude electron-hole pairing at this doping level.

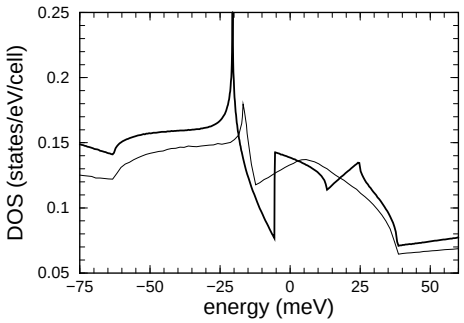

FIG. 1. The density of states in SrB_6 for two types of interband hybridization (a) isotropic excitonic gap, bold line, and (b) anisotropic crystal-field mixing Eq. (1), thin line.

(iv) Nesting of electron pockets between inequivalent X-points was suggested in Ref. [1] as another source of CDW and SDW instabilities, which does not involve holes from the valence band. This suggestion is physically incorrect. The nesting condition refers to a sign change under translation in momentum space: $\epsilon(k+Q) \approx -\epsilon(k)$. Only in such a case can repulsive *e-e* interaction produce a density-wave instability in *e-h* channel, see e.g. [7].

Lastly, the interpretation of the de Haas-van Alphen measurements quoted in [1] seems to us to be problematic in view of the high values of the low temperature resistivity reported for SrB_6 [8] and its strong dependence on stoichiometry. Further information is required before a definitive conclusion can be made.

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